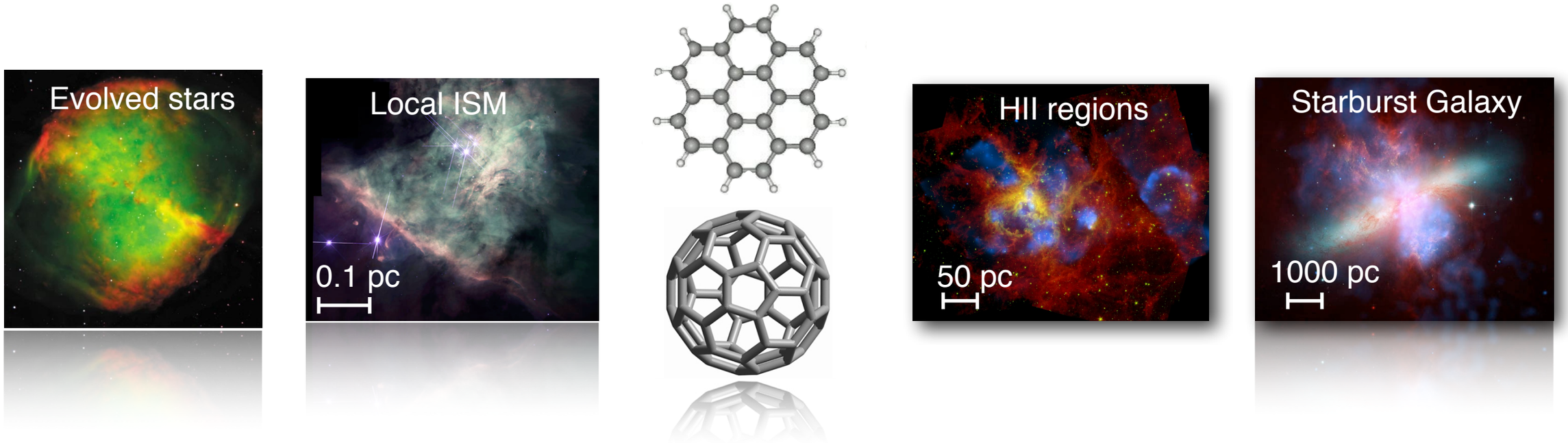
Data need for JWST
(…and E-ELT, ALMA/SKA/SPICA)

Jeronimo Bernard-Salas



Images credit: JK group (Cambridge), ESO, O'Dell & Wong, NASA, B.R. Brandl.

Belfast, April 2015

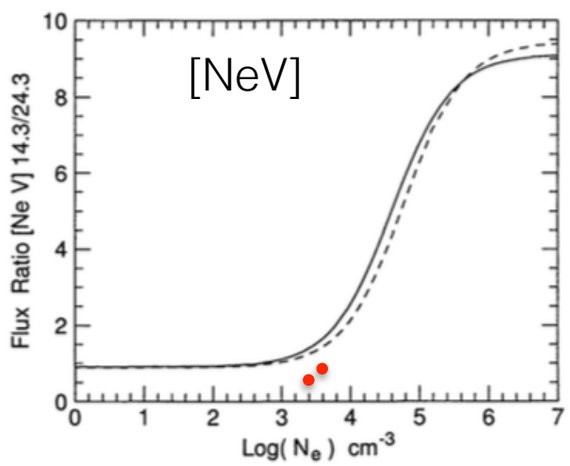
Summary

Atomic

- T_e, n_e, abundances

➡ TIPbase project. Overall happy with data in hand

- Ω_{col} for [NeV], resolve differences (e.g.[SIII], [NII])
- Old values, renew?



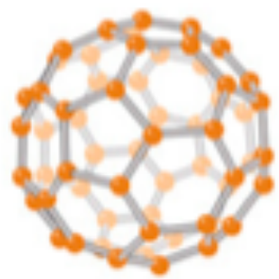
JWST

Molecular

- Excitation conditions

➡ UMIST, CDMS, JPL

- Collisional rates for CH^+ with H_2/e^- and OH with H_2



- Fullerenes: discrepancy relative strengths of C_{60}!

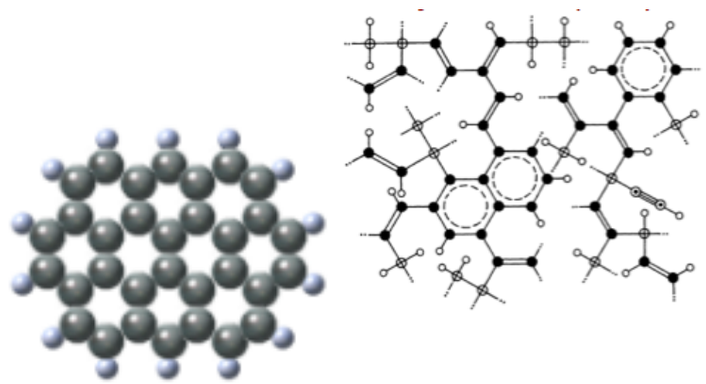
Herschel, ALMA, SKA, SPICA, JWST

PAHs/HAC/…

- Dust evolution, star formation tracers

➡ NASA Ames, Jena db

- Molecular physics of large aromatics
- Spectra of carbonaceous dust (HAC/soot…)



JWST, E-ELT

Atomic data

- Fundamental to all methods of measuring T_e, n_e, and abundances in gaseous nebulae
  - H, He recombination lines
  - Collisionally excited lines for heavy elements

IR lines: accurate abundance determination

- ISO/Spitzer: Local/nearby galaxies
- JWST: across and distant galaxies (diagnostic)

(A, Ω_{col})

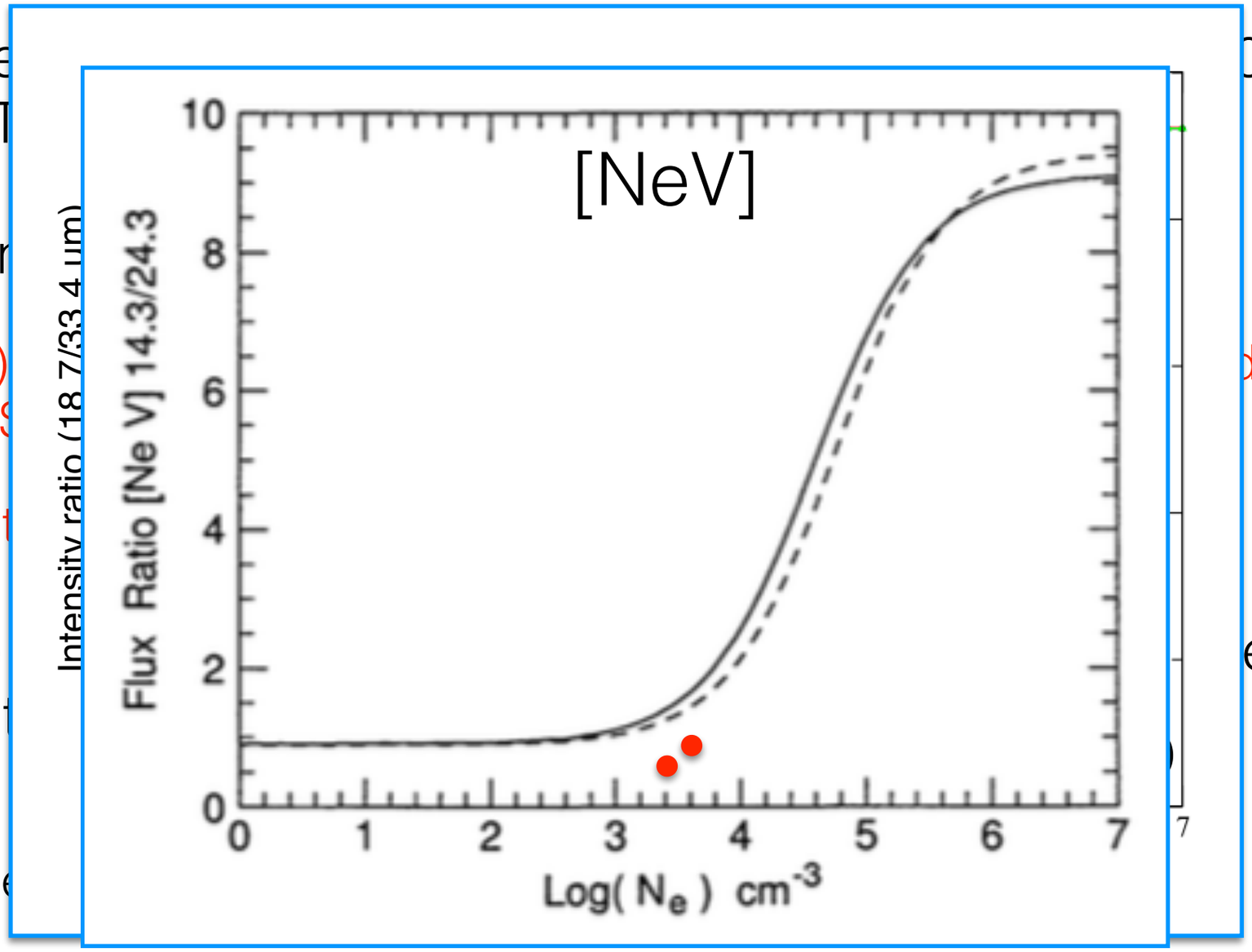
X Optical and UV
● ISO lines

Oxygen	Nitrogen	Carbon	Neon	Sulfur	Argon	Chlorine
O^+ X	N^+ X ●	C^+ X	Ne^+ ●	S^+ X	Ar^+ ●	Cl^+ X ●
O^{2+} X ●	N^{2+} X ●	C^{2+} X	Ne^{2+} X ●	S^{2+} X ●	Ar^{2+} X ●	Cl^{2+} X
O^{3+} X ●	N^{3+} X	C^{3+} X	Ne^{3+} X	S^{3+} ●	Ar^{3+} X	Cl^{3+} X ●
	N^{4+} X		Ne^{4+} X ●		Ar^{4+} X ●	Cl^{4+} ●
			Ne^{5+} ●		Ar^{5+} ●	

Magnesium	Silicon	Potassium	Aluminium	Calcium	Iron
Mg^+ X	Si^+ ●				Fe^+ ●
	Si^{2+} X	K^{2+} ●			Fe^{2+} ●
Mg^{3+} ●		K^{3+} X ●		Ca^{3+} ●	Fe^{3+} X
Mg^{4+} ●			Al^{4+} ●	Ca^{4+} X ●	Fe^{4+} ●
	Si^{5+} ●	K^{5+} X ●	Al^{5+} ●		Fe^{5+} ●
Mg^{6+} ●	Si^{6+} ●	K^{6+} ●		Ca^{6+} ●	Fe^{6+} ●
Mg^{7+} ●			Al^{7+} ●	Ca^{7+} ●	
	Si^{8+} ●				

Atomic data

- TIPbase
- Collisio
  - [NeV])
  - Uncert
- We use
  distribut
  - Could
    betwee



000 K. Also

different values

old…

ectron energy

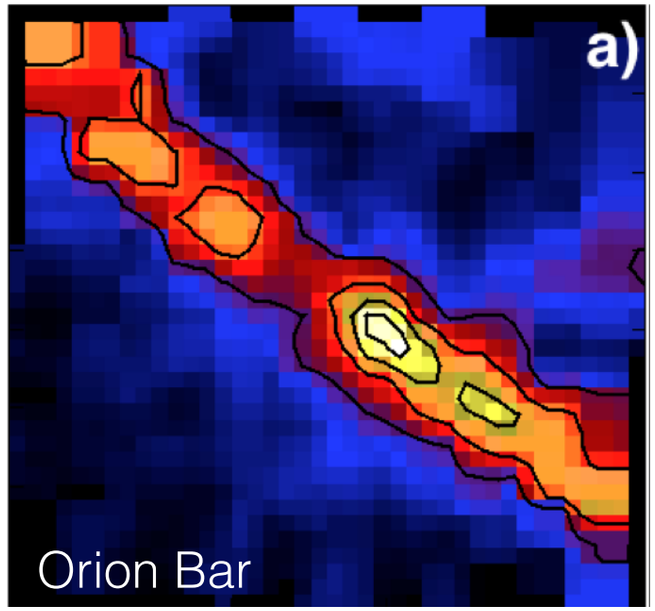
difference

C,N,O,Ne, S, Ar, Mg, Fe (Cl) — II, III, IV, V, VI — 5 level

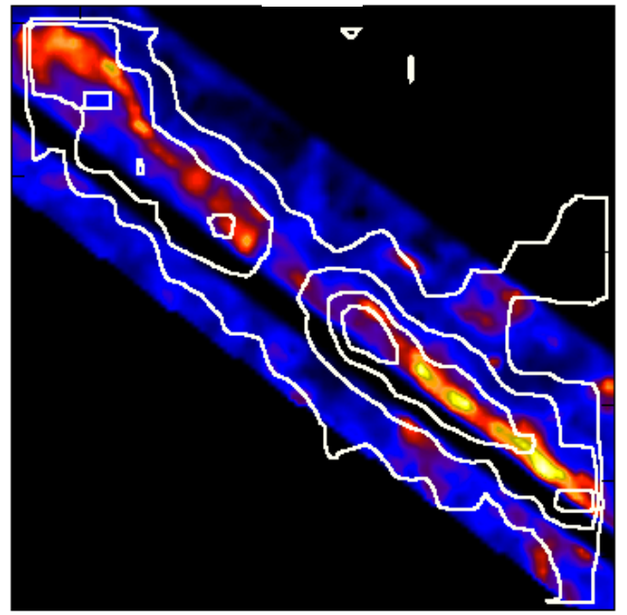
Molecules: OH, CH^+

- Key molecules tracing warm & dense phase of the ISM, also observed in diffuse ISM
- Important to constrain their formation and **excitation**!
- We use codes (Meudon, RADEX) which take UMIST, CDMS, JPL databases (CASSIS)
- **We need** collision rates: CH^+ with H_2 and e^-, and OH with e^-, for 10 <T< 2,000 K
- Now detected extragalactic environments!

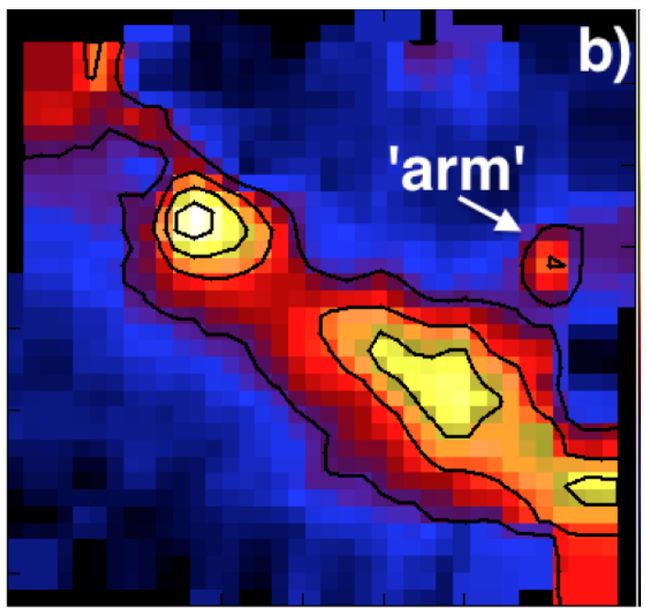
CH^+ J=3-2

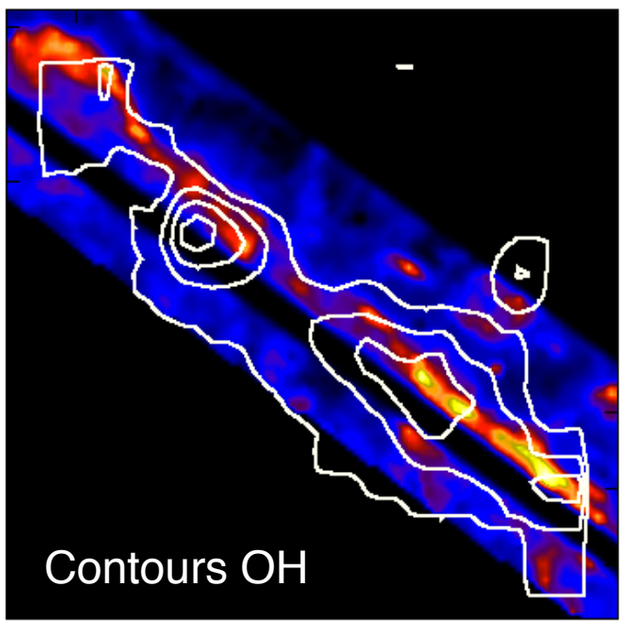


H2



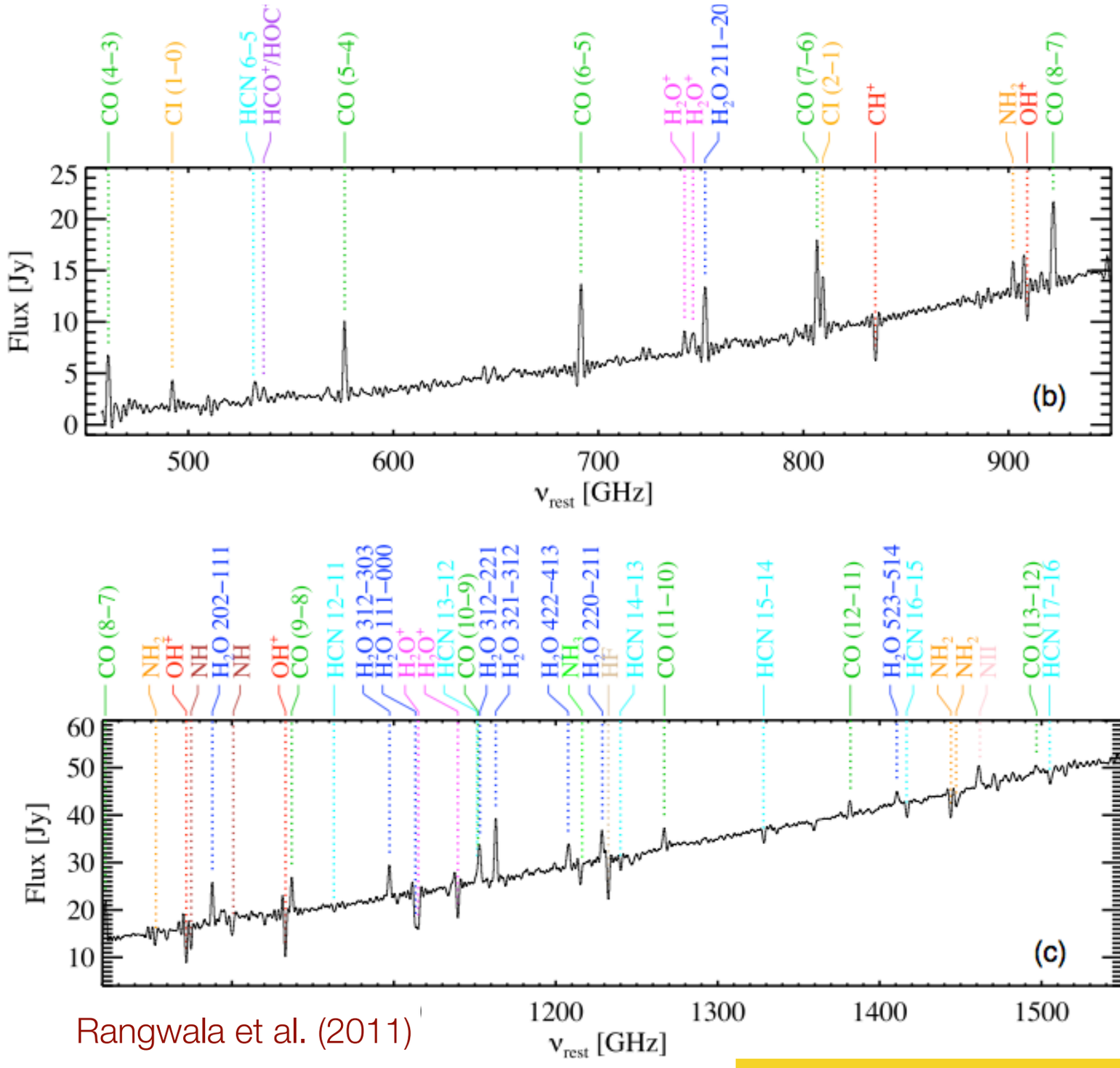
OH 84.6μm





Parikka et al. (2015)

Extragalactic



Rangwala et al. (2011)

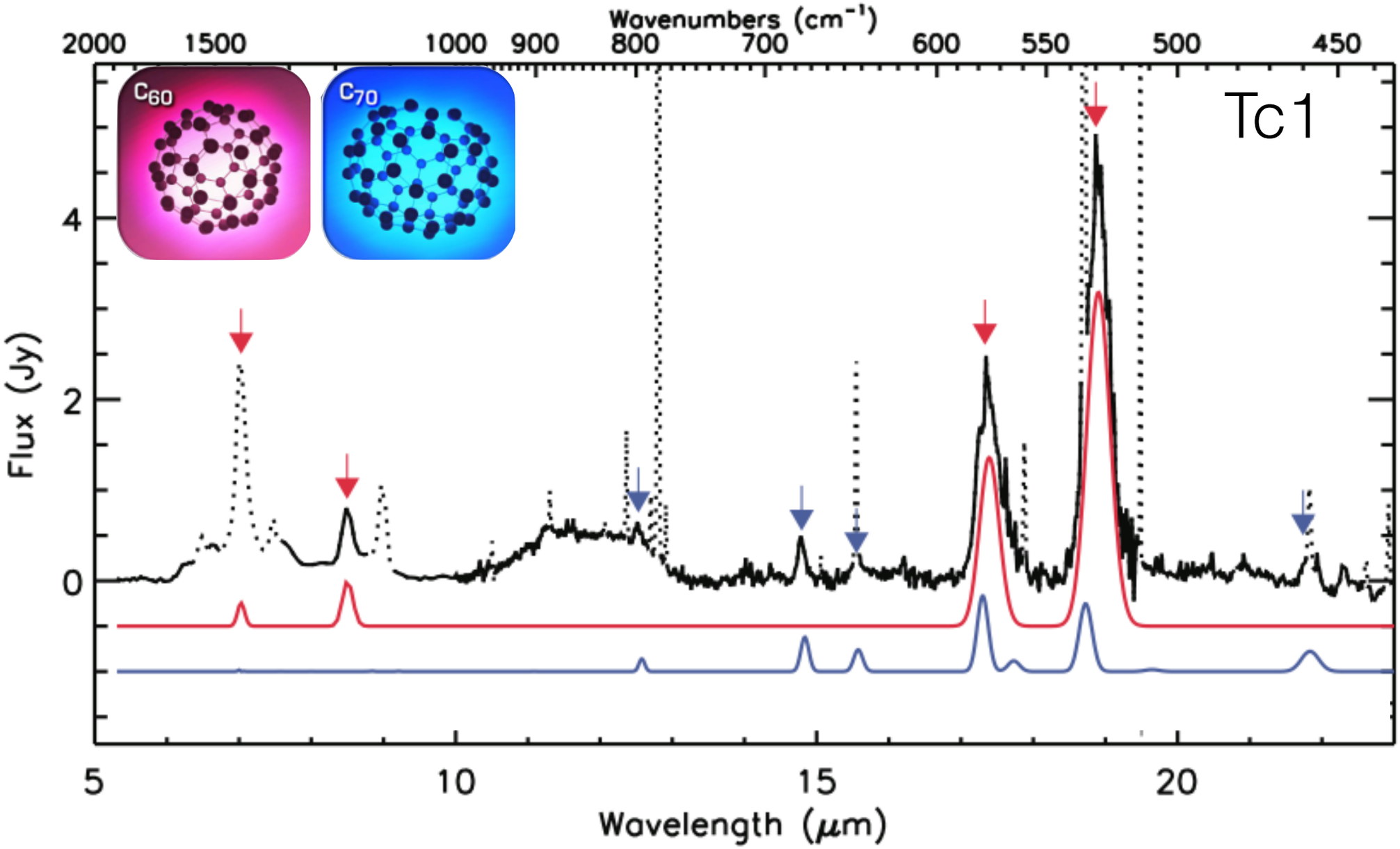
NH_2
OH^+
H_2O
HCN
NH_3
NH_2
HF
CH^+
H_2O
HCO
HCN
CO

Arp220
M82
NGC253
Mrk231
NGC4418
NGC1086
NGC6240
…

Growth area for:
ALMA
SKA
SPICA…

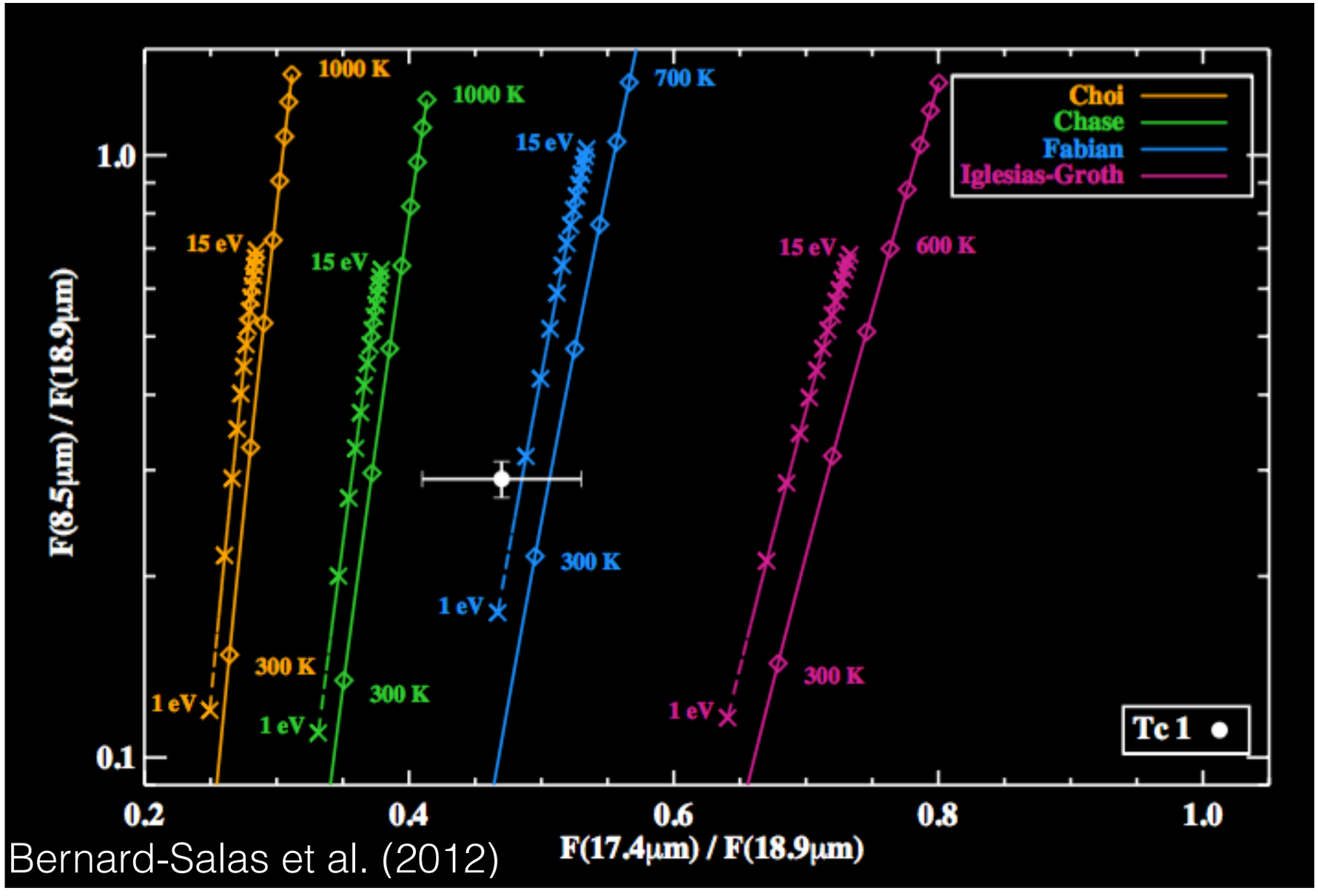
OH, OH^+ , CH^+, H_2O, HCN, HNC, CS, HF…

Fullerenes



Cami, Bernard-Salas et al. (2010, Science)

What is going on?



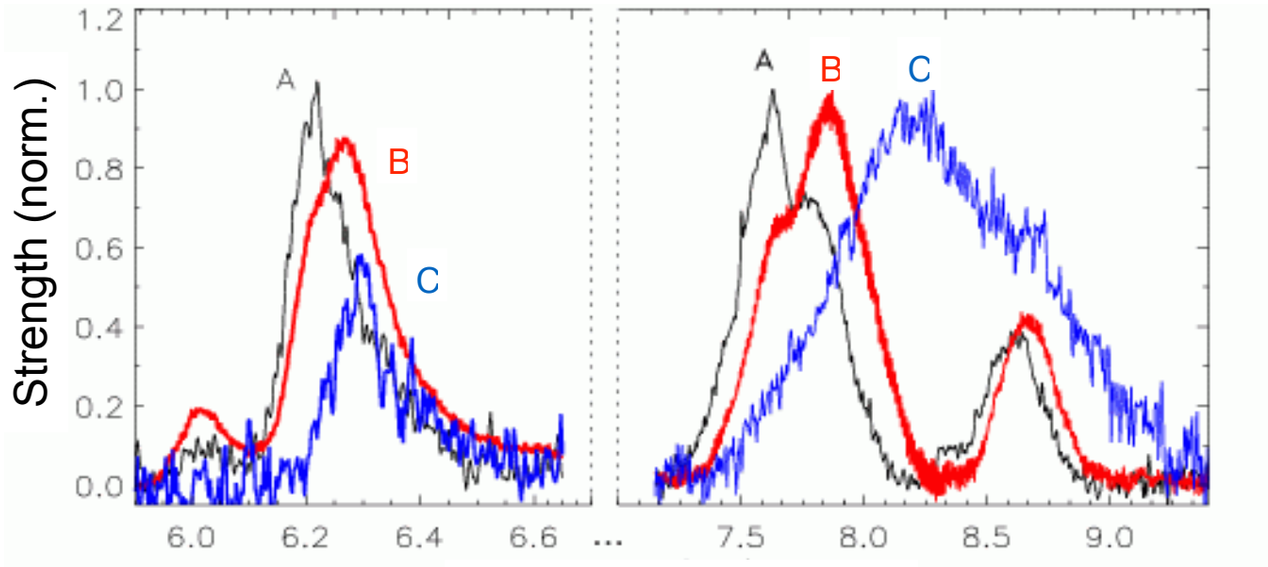
Bernard-Salas et al. (2012)

- We need reliable relative strength of the C_{60} bands
- Also, what is the effect of ^{13}C in spectra?

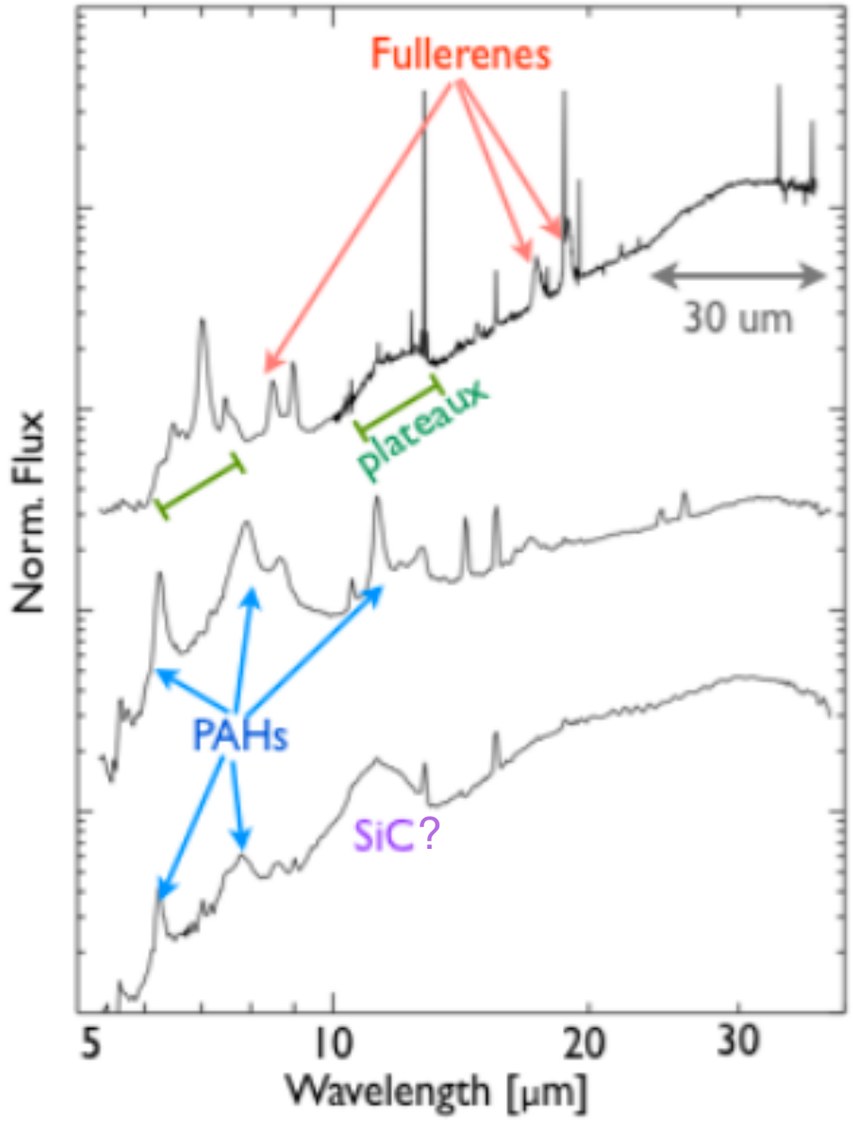
JWST

UIB - (PAHs, HAC, …)

- Rich (unidentified) chemistry in evolved stars
- PAHs ubiquitous in the Universe, vary in profile relative strength, peak position
- HAC: key element in linking these features



Peeters et al. (2003)



Bernard-Salas et al. (2012)

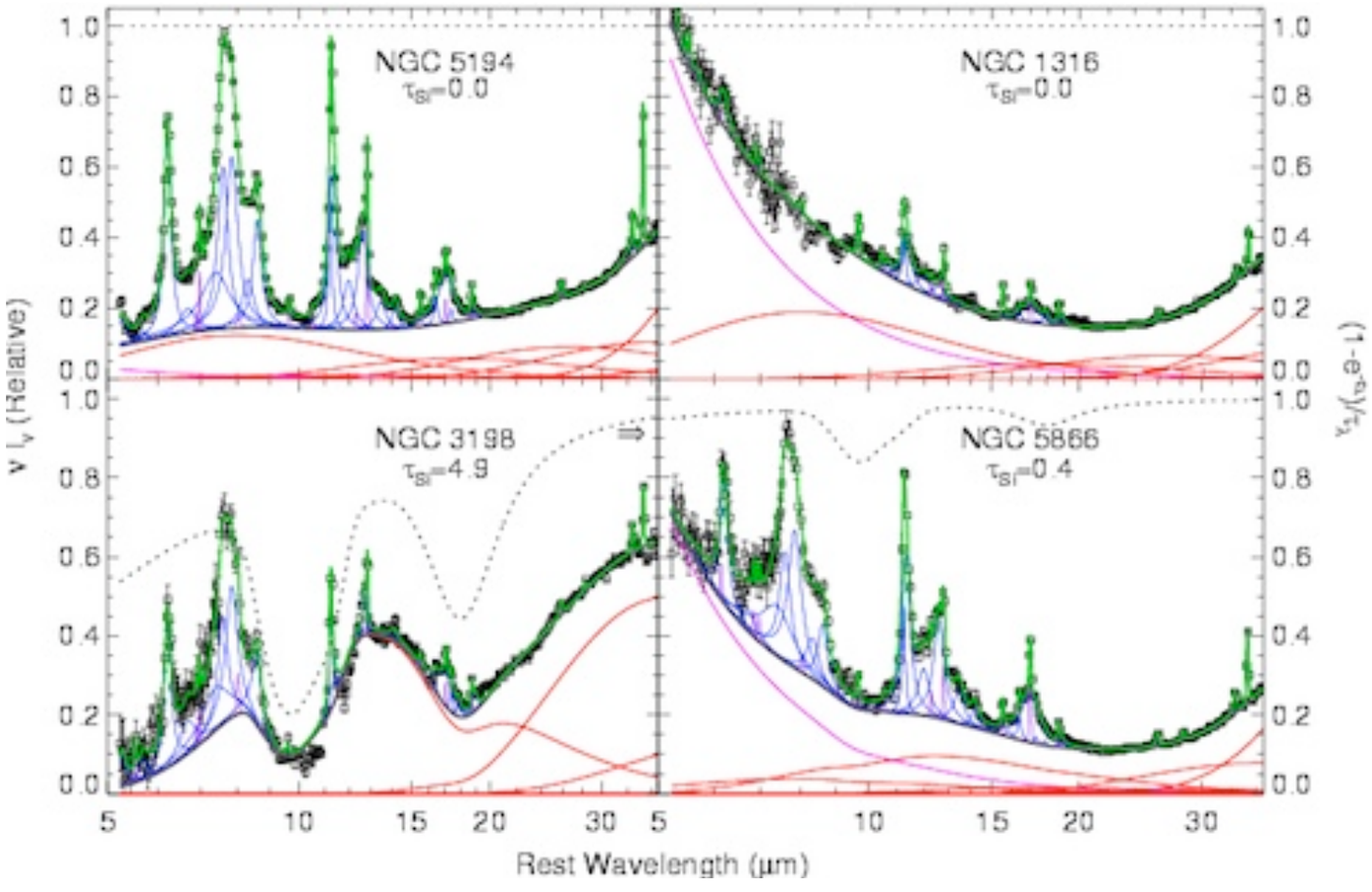
JWST spatially resolved studies of mid-IR in proto-planetary discs, and detect PAHs z~3.7, evolved stars up to the Virgo cluster

PAHs

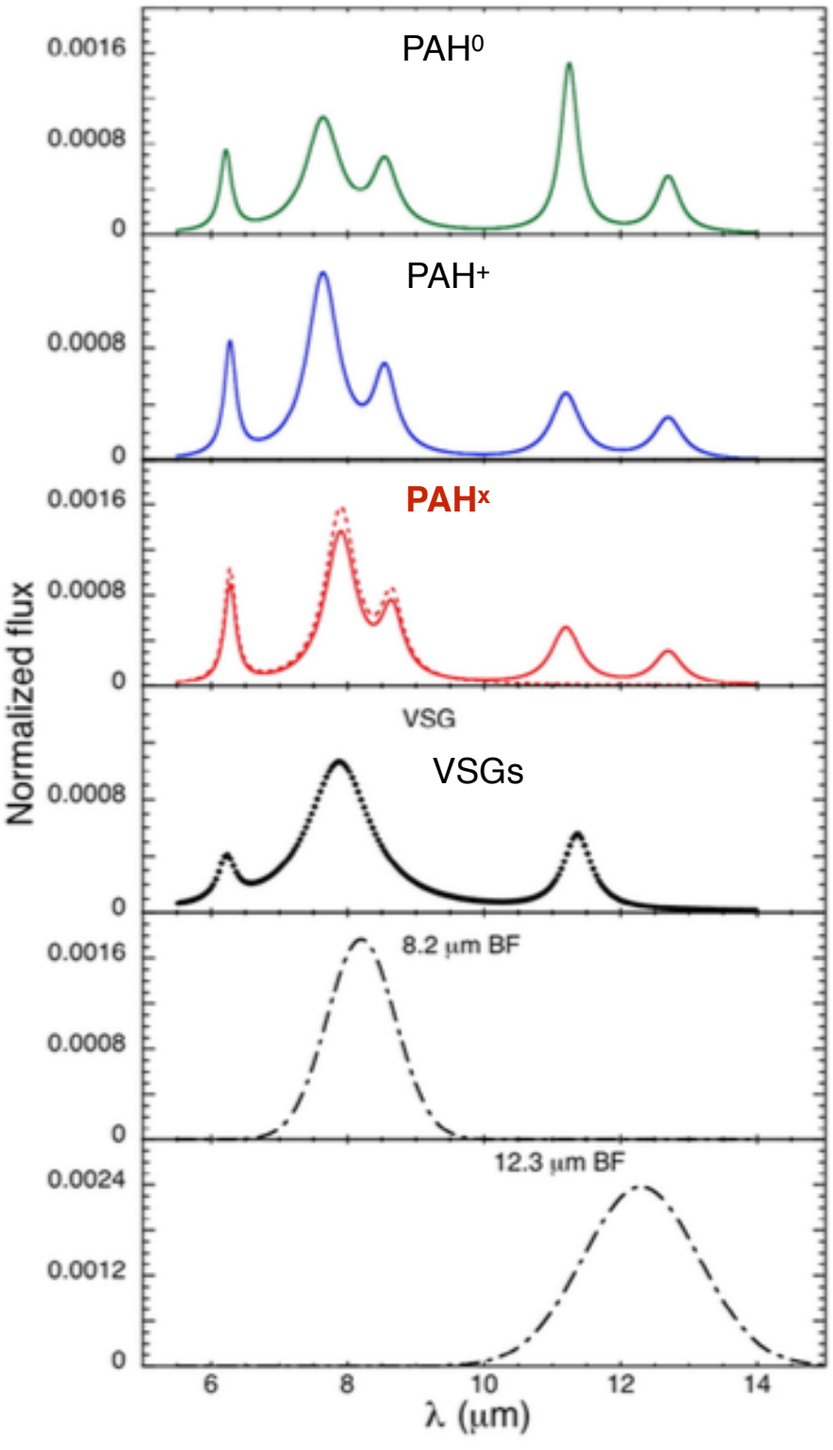
- Direct measurements from spectra or decomposition methods

PAHFIT

Smith et al. (2007)



- Best use spectral fits based on experimental or computational data *(e.g. PAH, NASA-Ames)*

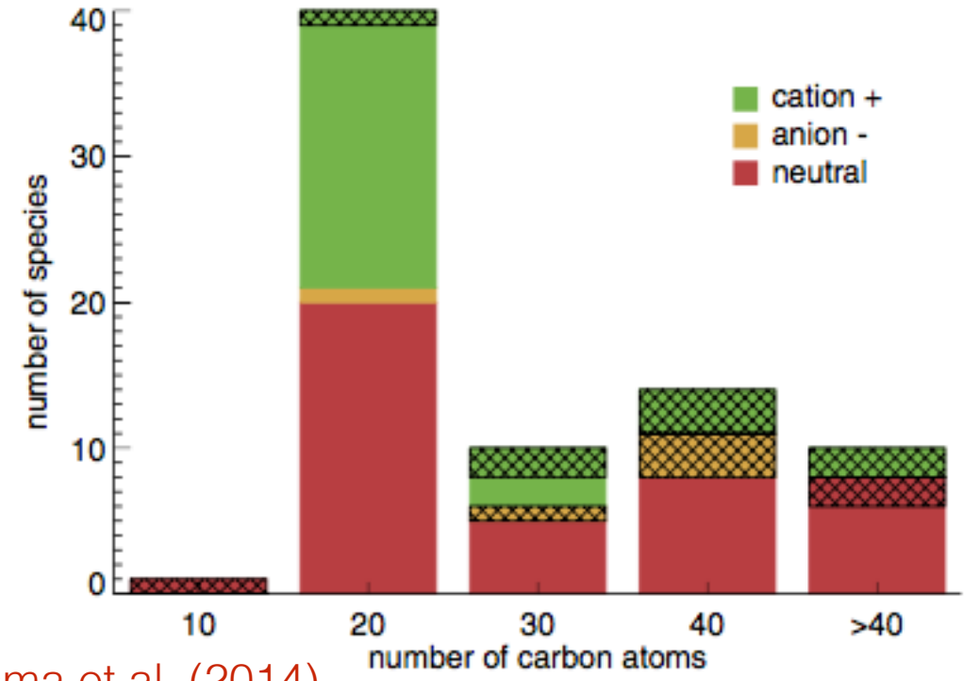


Joblin et al. (2008)

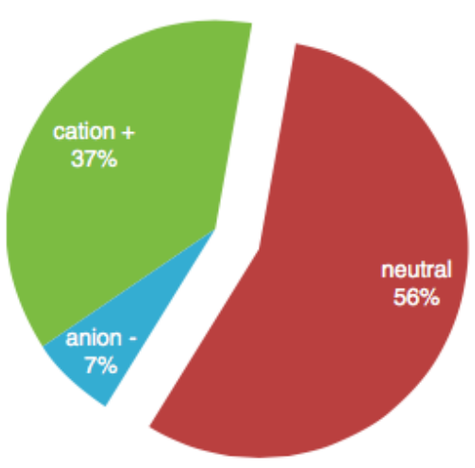
PAHs - NASA database

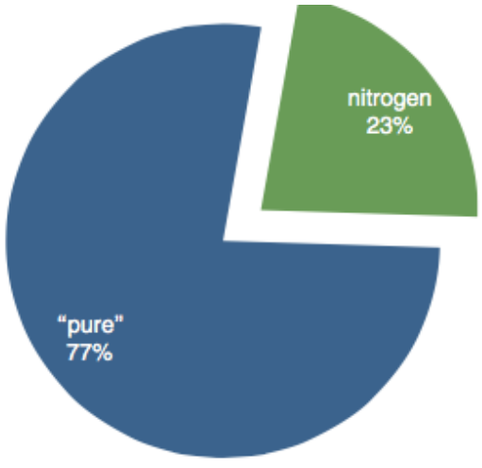
AmesPAHIDLdbSuite

Experimental

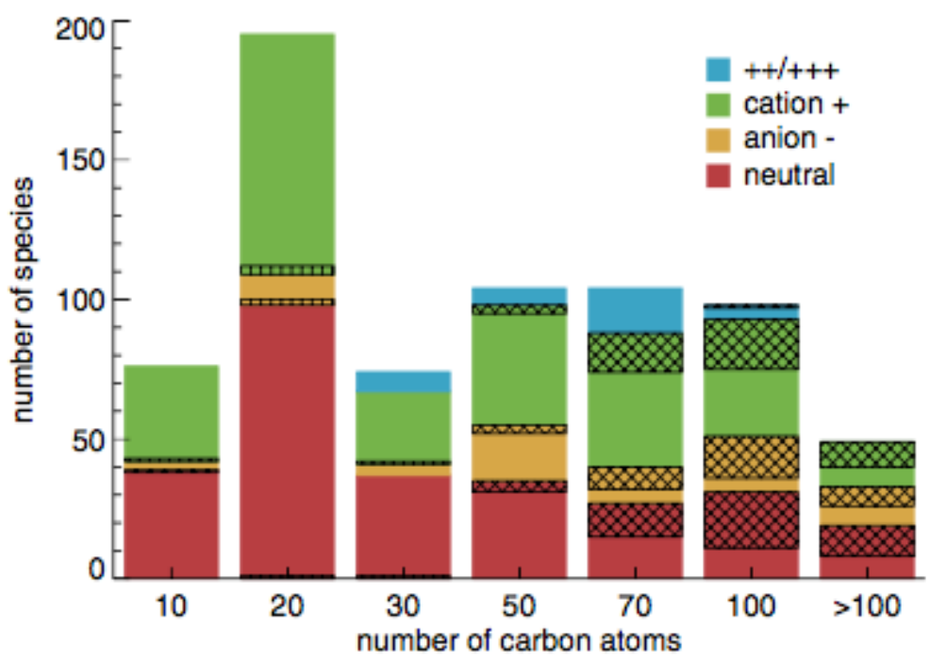


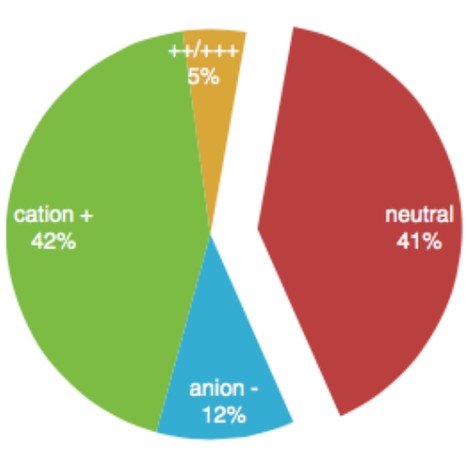
Boersma et al. (2014)

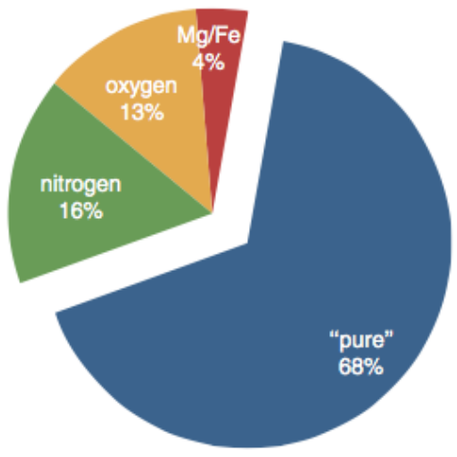




Computational



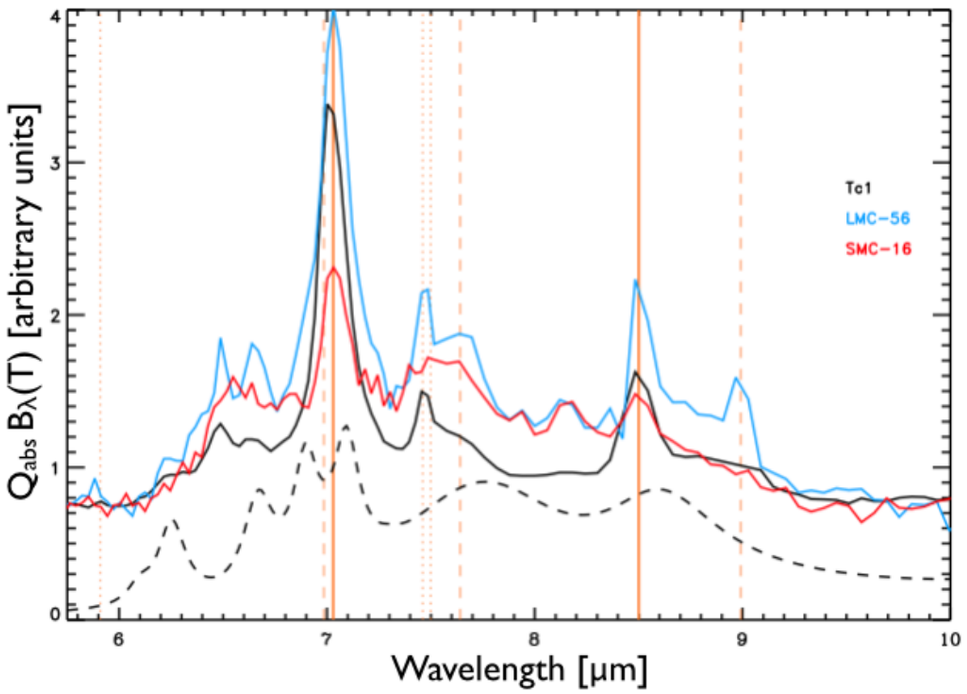




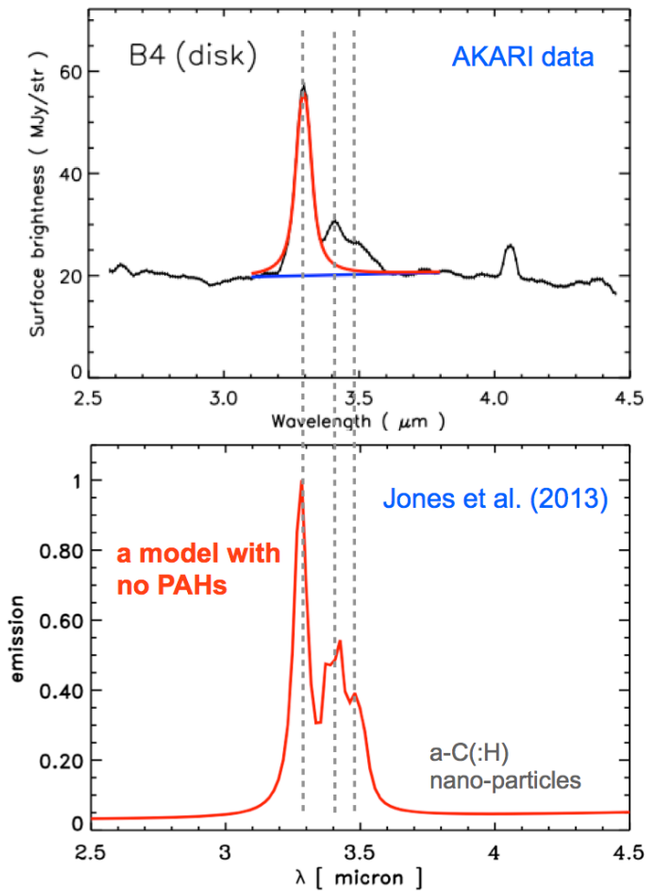
- Need experiments for larger PAHs (>40) and >3+ charge states for large PAHs
- *Molecular physics of large aromatics (high energy, anharmonicities, fragmentation)*

HAC, soot,…

- Use Jena database, Menella, Zubko…
- Optical properties of c-material at longer wavelength (>6um) not well characterised
- We do not have a good idea of how soot, clusters look like



Bernard-Salas et al. (2012)



- E-ELT will offer to study the aliphatic-aromatic components in the 3um region

➡ Ideally we want gas-phase optical properties of PAHs, HAC

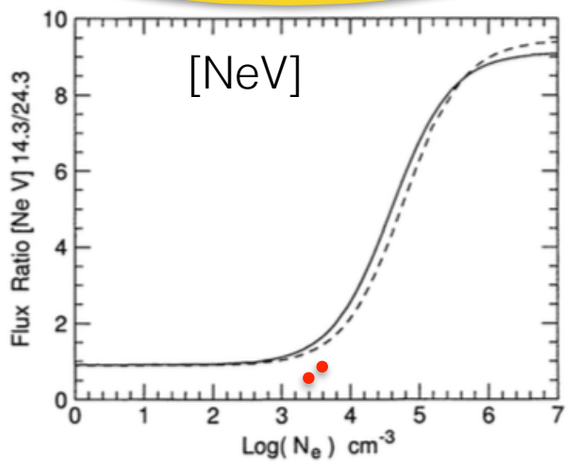
Summary

Atomic

- T_e, n_e, abundances

➡ TIPbase project. Overall happy with data in hand

- Different Ω_{col} for some ions e.g.[SIII], [NII], [NeV]
- Old values, uncertainties?



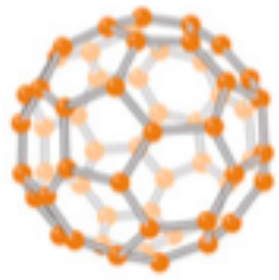
JWST

Molecular

- Excitation conditions

➡ UMIST, CDMS, JPL

- Collisional rates for CH^+ &with H_2/e-OH and OH with H_2



- Fullerenes: discrepancy relative strengths of C_{60}!

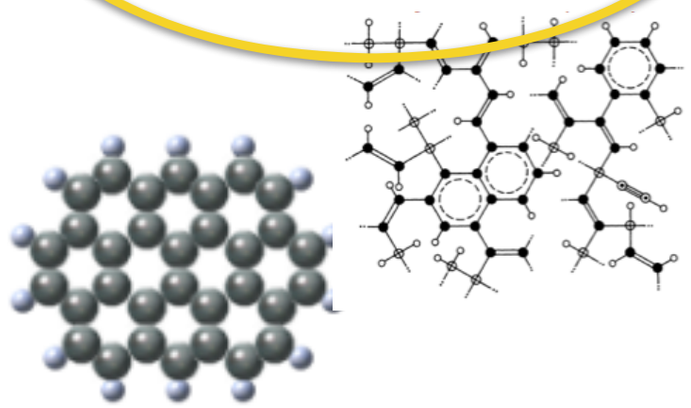
ALMA, SKA, JWST, SPICA

PAHs/HAC/…

- Dust evolution, star formation tracers

➡ NASA Ames database

- Molecular physics of large aromatics
- Spectra of carbonaceous dust (HAC/soot…)



JWST, E-ELT